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LLNL's Program on Multiscale Modeling of Polycrystal Plasticity

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Since the development of quantum mechanics great strides have been made in understanding materials phenomena based on "first principles" associated with atomic and sub-atomic structure. Perhaps the most notable examples are in the fields of microelectronics and nuclear energy. In other fields the connections between the fundamental nature of atomic structure and important properties are problematic because in addition to atomic structure, other structural aspects of the material at longer length scales are important. This is the case when considering the mechanical behavior of metals. Although general relationships between composition of metals and their mechanical properties have been established, a detailed understanding of the effects of the composition and microstructure based on first principles is lacking. For example, it is well known that a metal's strength increases if the grain size is decreased (the well documented Hall-Petch effect), however there is no fundamental understanding of this phenomenon.

In recent years there has been increasing interest in using what are termed "multiscale modeling" approaches to understand the effects of composition and microstructure on mechanical behavior. Two fundamental approaches have emerged. The first is essentially a nesting of an atomistic simulation in a continuum computer code simulation; this approach has been used to relate the propagation of cracks to the atomic structure at crack tips. The second approach to multiscale modeling is based on information-passing between different simulations at various length scales which capture all of the relevant material behavior, as shown in Figure 1. In this approach there is a decoupling of length and time scale and, in principle, macroscopic behavior such as a metal forming operation can ultimately be modeled with continuum computer codes with no decrease in computational efficiency.

At LLNL a multiscale modeling program based on information-passing has been established for modeling the strength properties of a body-centered-cubic metal (tantalum) under conditions of extreme plastic deformation. The plastic deformation experienced by an explosively-formed shaped-charge jet, shown in Figure 2, is an example of "extreme deformation". The shaped charge liner material undergoes high strain rate deformation at high hydrostatic pressure. The constitutive model for flow stress, which describes the deformation, is highly dependent on pressure, temperature, and strain-rate. Current material models can not be extrapolated to these extreme conditions because the underlying mechanisms of plastic deformation are poorly reflected in the models and laboratory experiments are limited to pressures orders of magnitude less than actual pressures. This disparity between actual deformation conditions and those that can be attained in laboratory experiments is the principle motivation behind the multiscale modeling program.

The fundamental elements of LLNL's multiscale modeling program are distinct models at the atomistic, microscale and mesoscale/continuum length scales. The information that needs to be passed from the lower to higher length scales (summarized in Figure 1) has been carefully defined to bound the levels of effort required to "bridge" length scales. Information that needs to be generated by the different simulations has been specified by a multidisplinary steering group comprised of physicists, materials scientists and engineers. The ultimate goal of the program is to provide critical information on strength properties to be used in continuum computer code simulations. The technical work-plan involves three principle areas which are highly coupled: 1) simulation development, 2) deformation experiments and 3) characterizations of deformed crystals. The three work areas are presented which provide examples of the progress of LLNL's program.

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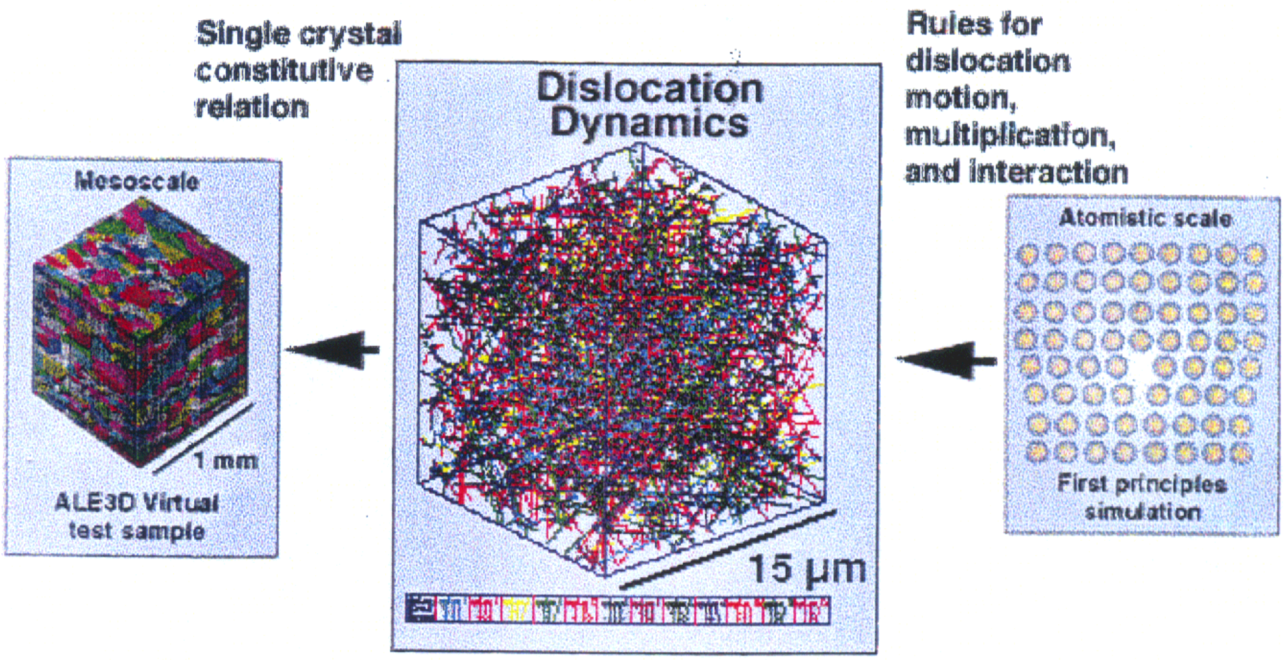

Figure 1. LLNL's multiscale modeling program is based on three key simulations and information passing .

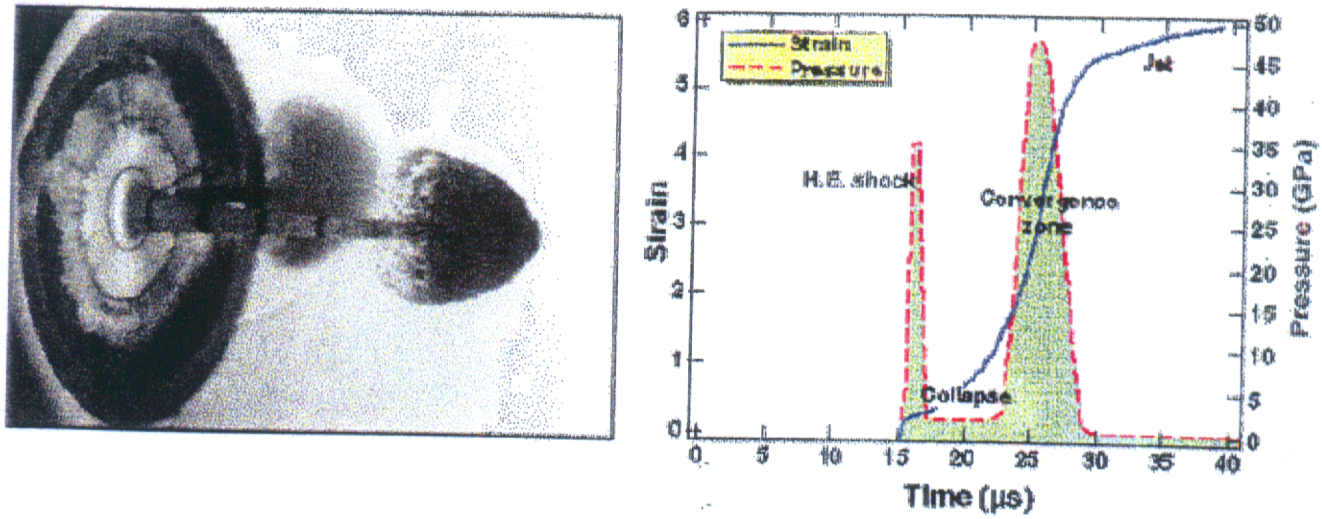

Figure 2. Predictive strength models are required for computer code simulations involving combinations of high strain rate deformation under high hydrostatic loading.